



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 08:32 pm BST

PDB ID : 5GTL
Title : NADPH complex structure of Aldehyde Dehydrogenase from Bacillus cereus
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Deposited on : 2016-08-21
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

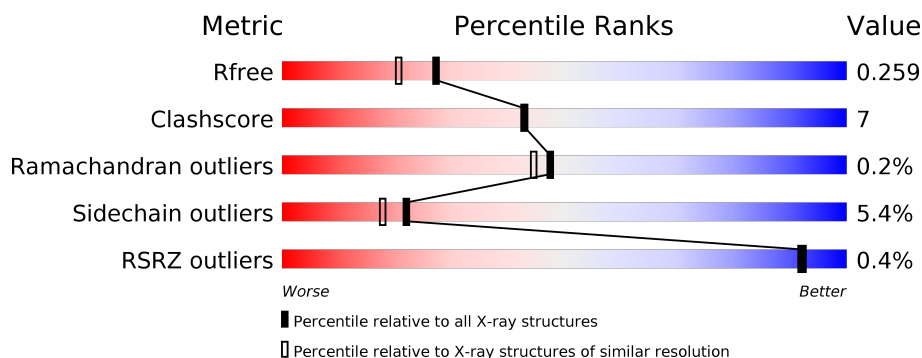
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	494	 86% 12% ..
1	B	494	 86% 13% ..
1	C	494	 79% 18% ..
1	D	494	 82% 15% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16824 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

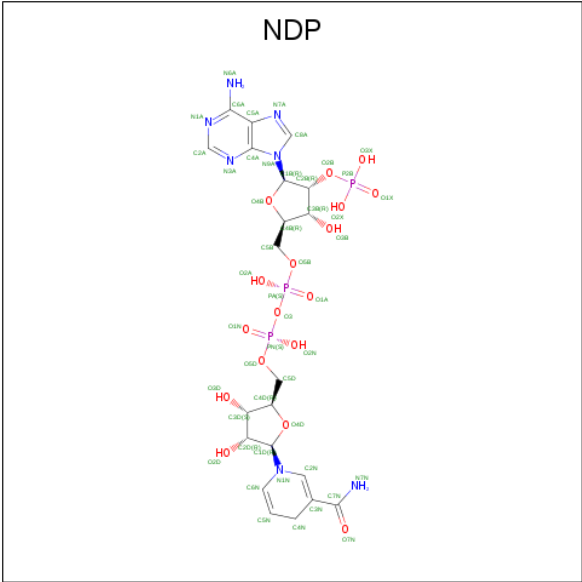
- Molecule 1 is a protein called Betaine-aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	0	0	0
			3791	2414	630	733	14			
1	B	491	Total	C	N	O	S	0	0	0
			3791	2414	630	733	14			
1	C	488	Total	C	N	O	S	0	0	0
			3768	2400	626	728	14			
1	D	489	Total	C	N	O	S	0	0	0
			3776	2406	627	729	14			

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Na	0	0
			2	2		
2	A	2	Total	Na	0	0
			2	2		
2	D	1	Total	Na	0	0
			1	1		
2	C	2	Total	Na	0	0
			2	2		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

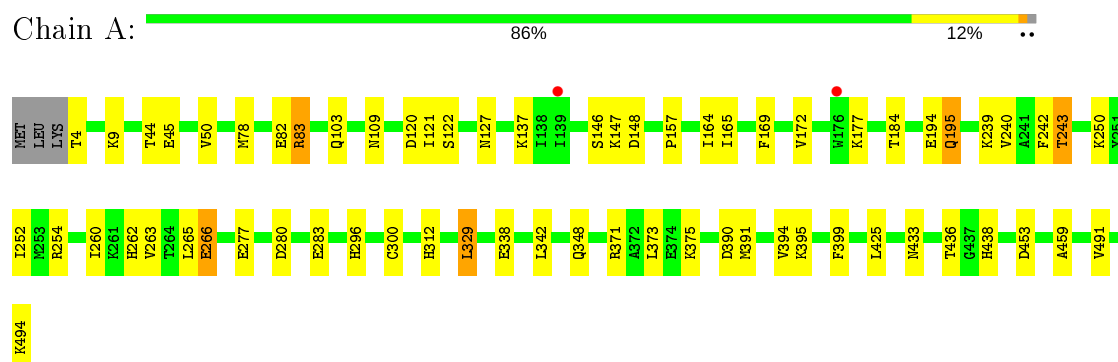
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	454	Total	O	0	0
			454	454		
4	B	421	Total	O	0	0
			421	421		
4	C	291	Total	O	0	0
			291	291		
4	D	333	Total	O	0	0
			333	333		

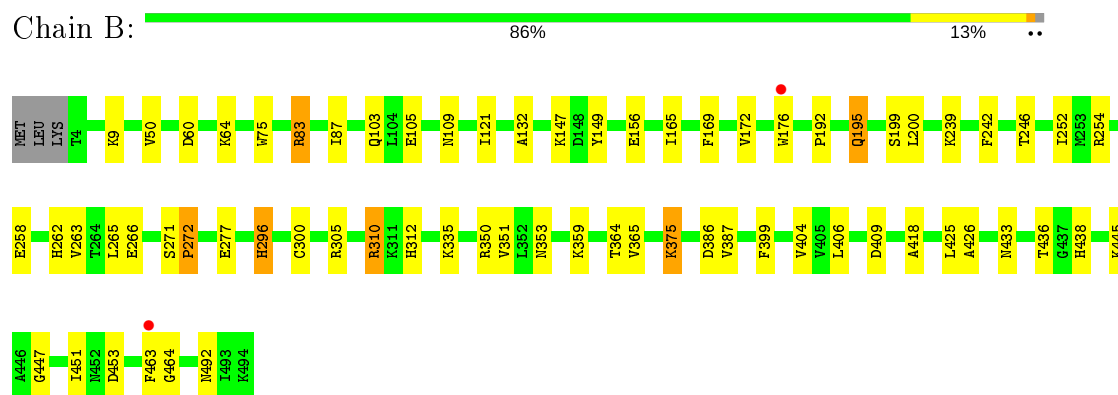
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

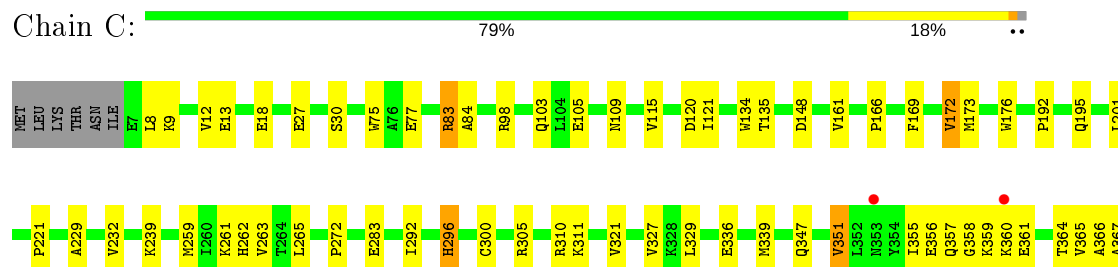
• Molecule 1: Betaine-aldehyde dehydrogenase



• Molecule 1: Betaine-aldehyde dehydrogenase

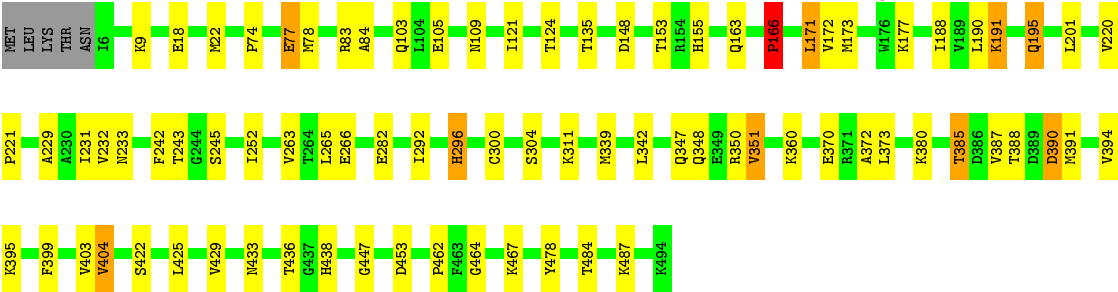
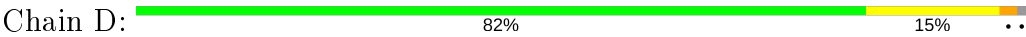


• Molecule 1: Betaine-aldehyde dehydrogenase





● Molecule 1: Betaine-aldehyde dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.89Å 93.94Å 144.93Å 90.00° 97.67° 90.00°	Depositor
Resolution (Å)	47.88 – 2.00 47.88 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.88-2.00) 99.9 (47.88-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.91 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.189 , 0.252 0.203 , 0.259	Depositor DCC
R_{free} test set	7525 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16824	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, NA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.23	1/3870 (0.0%)	0.98	4/5250 (0.1%)
1	B	1.22	2/3870 (0.1%)	0.99	4/5250 (0.1%)
1	C	1.08	0/3847	0.96	2/5218 (0.0%)
1	D	1.12	0/3855	0.97	2/5229 (0.0%)
All	All	1.16	3/15442 (0.0%)	0.97	12/20947 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	156	GLU	CD-OE2	-6.02	1.19	1.25
1	A	338	GLU	CD-OE1	-5.83	1.19	1.25
1	B	199	SER	CB-OG	-5.24	1.35	1.42

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	305	ARG	NE-CZ-NH1	8.94	124.77	120.30
1	B	83	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	B	305	ARG	NE-CZ-NH2	-7.29	116.66	120.30
1	B	254	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	A	254	ARG	NE-CZ-NH1	6.71	123.65	120.30
1	D	83	ARG	NE-CZ-NH1	-5.94	117.33	120.30
1	D	148	ASP	CB-CG-OD1	5.46	123.21	118.30
1	A	83	ARG	NE-CZ-NH2	5.39	122.99	120.30
1	C	305	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	A	329	LEU	CA-CB-CG	5.27	127.42	115.30
1	A	148	ASP	CB-CG-OD1	5.15	122.94	118.30
1	C	400	GLY	N-CA-C	-5.11	100.33	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3791	0	3740	51	0
1	B	3791	0	3740	44	0
1	C	3768	0	3716	58	0
1	D	3776	0	3727	66	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	1	0	0	1	0
3	A	48	0	26	1	0
3	B	48	0	26	0	0
3	C	48	0	26	0	0
3	D	48	0	26	4	0
4	A	454	0	0	6	0
4	B	421	0	0	6	0
4	C	291	0	0	10	0
4	D	333	0	0	8	0
All	All	16824	0	15027	207	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (207) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:351:VAL:O	1:C:355:ILE:HD12	1.32	1.28
1:C:391:MET:SD	4:C:806:HOH:O	2.00	1.17
1:D:347:GLN:O	1:D:351:VAL:HG12	1.66	0.95
1:A:195:GLN:H	1:A:195:GLN:HE21	1.22	0.86
1:D:385:THR:HG21	4:D:883:HOH:O	1.76	0.85
1:D:342:LEU:CD1	1:D:351:VAL:HG11	2.06	0.85
1:B:375:LYS:HE3	4:B:671:HOH:O	1.76	0.84
1:C:351:VAL:O	1:C:355:ILE:CD1	2.24	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:GLU:HG2	4:A:968:HOH:O	1.78	0.82
1:C:18:GLU:HG3	4:C:764:HOH:O	1.79	0.80
1:C:387:VAL:HA	4:C:806:HOH:O	1.84	0.76
1:B:83:ARG:HD3	4:B:614:HOH:O	1.85	0.76
1:D:9:LYS:H	1:D:103:GLN:HE22	1.34	0.75
1:B:239:LYS:HZ3	1:B:262:HIS:HD2	1.31	0.74
1:B:195:GLN:H	1:B:195:GLN:HE21	1.36	0.74
1:C:148:ASP:HB3	1:C:494:LYS:HG3	1.71	0.72
1:D:84:ALA:HB2	1:D:135:THR:OG1	1.91	0.70
1:C:84:ALA:HB2	1:C:135:THR:OG1	1.91	0.70
1:B:165:ILE:HD11	4:B:859:HOH:O	1.91	0.70
1:B:438:HIS:HE1	1:C:438:HIS:HE1	1.41	0.69
1:A:243:THR:HG21	4:A:636:HOH:O	1.93	0.68
1:C:300:CYS:SG	1:C:425:LEU:HD21	2.34	0.68
1:C:192:PRO:HA	4:C:605:HOH:O	1.94	0.67
1:D:347:GLN:O	1:D:351:VAL:CG1	2.41	0.67
1:C:169:PHE:HB3	1:C:172:VAL:HG22	1.75	0.67
1:C:9:LYS:H	1:C:103:GLN:HE22	1.44	0.66
1:D:370:GLU:O	1:D:380:LYS:HG3	1.96	0.66
1:D:467:LYS:O	4:D:603:HOH:O	2.15	0.65
1:D:388:THR:OG1	4:D:602:HOH:O	2.14	0.65
1:A:169:PHE:HB3	1:A:172:VAL:CG1	2.27	0.64
1:B:9:LYS:H	1:B:103:GLN:HE22	1.43	0.64
1:B:350:ARG:NH1	4:B:601:HOH:O	2.31	0.63
1:C:83:ARG:HG3	1:C:83:ARG:HH11	1.65	0.62
1:C:387:VAL:HG12	4:C:806:HOH:O	2.00	0.61
1:D:342:LEU:HD11	1:D:351:VAL:HG11	1.81	0.60
1:A:9:LYS:H	1:A:103:GLN:HE22	1.49	0.60
1:D:229:ALA:HA	1:D:232:VAL:HG12	1.82	0.60
1:D:387:VAL:HG23	1:D:391:MET:SD	2.41	0.60
2:D:501:NA:NA	4:D:601:HOH:O	1.74	0.60
1:A:494:LYS:HE3	4:A:767:HOH:O	2.02	0.60
1:C:356:GLU:O	1:C:359:LYS:N	2.35	0.59
1:A:300:CYS:SG	1:A:425:LEU:HD21	2.43	0.59
1:C:8:LEU:HB3	1:C:13:GLU:HG3	1.83	0.59
1:A:391:MET:HB2	1:A:394:VAL:HG13	1.85	0.58
1:B:239:LYS:NZ	1:B:262:HIS:HD2	2.02	0.58
1:B:75:TRP:CH2	1:B:83:ARG:HD2	2.39	0.57
1:C:259:MET:HE3	1:C:261:LYS:HE3	1.85	0.57
1:C:355:ILE:HG21	1:C:369:GLY:HA2	1.86	0.57
1:A:177:LYS:HZ1	1:A:243:THR:CG2	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:433:ASN:HD22	1:D:436:THR:H	1.51	0.57
1:C:310:ARG:HD2	1:C:409:ASP:OD1	2.04	0.57
1:A:263:VAL:HG12	1:A:265:LEU:HG	1.86	0.56
1:D:387:VAL:CG2	1:D:391:MET:SD	2.93	0.56
1:A:240:VAL:CG1	1:A:263:VAL:HG22	2.35	0.56
1:C:347:GLN:O	1:C:351:VAL:HG13	2.04	0.56
1:B:438:HIS:HE1	1:C:438:HIS:CE1	2.24	0.56
1:D:350:ARG:HG2	1:D:350:ARG:HH11	1.68	0.56
1:C:173:MET:HG2	1:C:176:TRP:CZ3	2.42	0.55
1:B:239:LYS:HZ3	1:B:262:HIS:CD2	2.19	0.55
1:B:359:LYS:HE2	1:B:365:VAL:HG11	1.89	0.54
1:D:229:ALA:O	1:D:232:VAL:HG12	2.07	0.54
1:B:263:VAL:HG12	1:B:265:LEU:HG	1.89	0.54
1:A:438:HIS:CE1	1:D:438:HIS:HE1	2.25	0.54
1:D:22:MET:CG	1:D:221:PRO:HD2	2.37	0.54
1:C:388:THR:OG1	1:C:390:ASP:OD1	2.21	0.54
1:B:195:GLN:HG3	4:B:967:HOH:O	2.08	0.53
1:B:438:HIS:CE1	1:C:438:HIS:HE1	2.22	0.53
1:C:433:ASN:HD22	1:C:436:THR:H	1.57	0.53
1:A:195:GLN:H	1:A:195:GLN:NE2	2.01	0.53
1:A:239:LYS:HZ3	1:A:262:HIS:HD2	1.55	0.53
1:C:359:LYS:HE2	1:C:365:VAL:HG11	1.92	0.52
1:A:433:ASN:HD22	1:A:436:THR:H	1.58	0.52
1:D:242:PHE:CD1	1:D:252:ILE:HD13	2.45	0.52
1:D:342:LEU:HD13	1:D:351:VAL:HG11	1.91	0.52
1:C:272:PRO:HG3	1:C:418:ALA:HB1	1.91	0.52
1:D:245:SER:HB3	3:D:502:NDP:O4D	2.11	0.52
1:D:447:GLY:HA3	1:D:464:GLY:O	2.11	0.51
1:D:195:GLN:NE2	3:D:502:NDP:O1X	2.44	0.50
1:D:201:LEU:HD11	1:D:221:PRO:HG3	1.94	0.50
1:C:192:PRO:CA	4:C:605:HOH:O	2.56	0.50
1:A:300:CYS:HB2	1:A:425:LEU:CD2	2.41	0.50
1:D:191:LYS:HG2	1:D:220:VAL:O	2.11	0.50
1:A:147:LYS:HE2	1:D:77:GLU:HG3	1.93	0.49
1:A:78:MET:HG2	1:A:82:GLU:HB2	1.93	0.49
1:C:327:VAL:HG11	1:C:339:MET:HE3	1.94	0.49
1:D:163:GLN:NE2	1:D:177:LYS:HB3	2.27	0.49
1:A:277:GLU:O	1:A:312:HIS:HE1	1.95	0.49
1:B:239:LYS:NZ	1:B:262:HIS:CD2	2.80	0.49
1:C:229:ALA:HA	1:C:232:VAL:HG12	1.93	0.49
1:A:438:HIS:HE1	1:D:438:HIS:HE1	1.58	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:263:VAL:HG12	1:C:265:LEU:HG	1.94	0.49
1:A:4:THR:N	4:A:608:HOH:O	2.46	0.49
1:D:263:VAL:HG12	1:D:265:LEU:HG	1.95	0.49
1:D:390:ASP:CB	4:D:865:HOH:O	2.61	0.48
1:C:172:VAL:HG13	4:C:653:HOH:O	2.12	0.48
1:A:390:ASP:O	1:A:395:LYS:HE2	2.13	0.48
1:B:272:PRO:HG3	1:B:418:ALA:HB1	1.94	0.48
1:C:367:ALA:O	1:C:382:THR:HG23	2.13	0.48
1:A:242:PHE:CD1	1:A:252:ILE:CD1	2.97	0.48
1:C:75:TRP:CZ2	1:C:83:ARG:HD3	2.48	0.48
1:D:390:ASP:HB3	4:D:865:HOH:O	2.13	0.48
1:B:447:GLY:HA3	1:B:464:GLY:O	2.13	0.48
1:A:243:THR:HA	1:A:266:GLU:O	2.13	0.48
1:C:201:LEU:HD11	1:C:221:PRO:HG3	1.96	0.48
1:D:124:THR:HG21	1:D:171:LEU:HD13	1.95	0.47
1:A:147:LYS:HE2	1:D:77:GLU:CG	2.44	0.47
1:D:232:VAL:HG13	1:D:233:ASN:N	2.29	0.47
1:A:44:THR:O	1:A:45:GLU:HB2	2.14	0.47
1:D:296:HIS:N	1:D:296:HIS:CD2	2.80	0.47
1:A:240:VAL:HG12	1:A:263:VAL:HG22	1.97	0.47
1:B:195:GLN:CG	4:B:967:HOH:O	2.62	0.47
1:B:364:THR:OG1	1:B:386:ASP:OD2	2.23	0.47
1:D:191:LYS:NZ	3:D:502:NDP:O2X	2.48	0.47
1:B:310:ARG:HD2	1:B:409:ASP:OD1	2.15	0.47
1:D:394:VAL:HG22	1:D:404:VAL:HG11	1.97	0.47
1:A:177:LYS:NZ	1:A:243:THR:CG2	2.78	0.47
1:D:166:PRO:HD2	1:D:173:MET:SD	2.55	0.47
1:C:420:ASN:HB3	4:C:701:HOH:O	2.15	0.46
1:C:447:GLY:HA3	1:C:464:GLY:O	2.16	0.46
1:B:169:PHE:HB3	1:B:172:VAL:HG12	1.98	0.46
1:D:163:GLN:HB2	1:D:190:LEU:HD23	1.98	0.46
1:D:242:PHE:CG	1:D:252:ILE:HD13	2.51	0.46
1:D:300:CYS:HB3	3:D:502:NDP:H72N	1.80	0.46
1:C:412:GLU:CD	1:C:412:GLU:H	2.19	0.46
1:A:312:HIS:HD2	4:A:928:HOH:O	1.97	0.46
1:C:391:MET:CE	4:C:806:HOH:O	2.54	0.46
1:D:74:PRO:O	1:D:78:MET:HB2	2.14	0.46
1:A:194:GLU:HG2	1:A:195:GLN:NE2	2.31	0.46
1:B:296:HIS:N	1:B:296:HIS:CD2	2.82	0.46
1:C:12:VAL:HG21	1:C:103:GLN:HE21	1.80	0.46
1:D:292:ILE:HG21	1:D:403:VAL:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:365:VAL:O	1:C:365:VAL:HG23	2.16	0.45
1:C:263:VAL:CG1	1:C:265:LEU:HD21	2.47	0.45
1:B:75:TRP:CH2	1:B:83:ARG:CD	3.00	0.45
1:A:169:PHE:HB3	1:A:172:VAL:HG12	1.99	0.45
1:A:239:LYS:NZ	1:A:262:HIS:HD2	2.13	0.45
1:A:78:MET:HG2	1:A:82:GLU:CB	2.46	0.45
1:B:404:VAL:HG23	1:B:406:LEU:HD11	1.98	0.45
1:C:321:VAL:HG21	1:C:366:ALA:HB1	1.99	0.45
1:D:300:CYS:SG	1:D:425:LEU:HD21	2.57	0.45
1:A:491:VAL:HG22	1:B:451:ILE:HD12	1.99	0.45
1:B:242:PHE:CD1	1:B:252:ILE:CD1	3.00	0.45
1:D:296:HIS:CD2	1:D:339:MET:HG3	2.52	0.45
1:A:263:VAL:CG1	1:A:265:LEU:HG	2.46	0.45
1:C:404:VAL:HG23	1:C:404:VAL:O	2.15	0.45
1:C:473:ARG:CZ	4:C:691:HOH:O	2.64	0.45
1:D:342:LEU:HD12	1:D:348:GLN:HA	1.98	0.45
1:A:137:LYS:HE3	1:C:134:TRP:CD1	2.52	0.44
1:C:120:ASP:O	1:C:172:VAL:HG12	2.17	0.44
1:D:372:ALA:HB2	1:D:380:LYS:HG2	1.98	0.44
1:A:280:ASP:OD1	1:A:283:GLU:HG2	2.17	0.44
1:A:164:ILE:HD13	3:A:503:NDP:H2A	1.98	0.44
1:C:372:ALA:HB3	1:C:378:PHE:HB3	1.98	0.44
1:D:22:MET:HG2	1:D:221:PRO:HD2	1.97	0.44
1:D:292:ILE:HD13	1:D:304:SER:HA	1.99	0.44
1:B:300:CYS:SG	1:B:425:LEU:HD21	2.57	0.44
1:D:263:VAL:CG1	1:D:265:LEU:HD21	2.48	0.44
1:D:229:ALA:HA	1:D:232:VAL:CG1	2.47	0.43
1:B:149:TYR:CD1	1:B:492:ASN:HA	2.53	0.43
1:C:296:HIS:CD2	1:C:339:MET:HG3	2.53	0.43
1:D:166:PRO:HD3	1:D:243:THR:HB	2.01	0.43
1:B:192:PRO:HG3	1:B:200:LEU:HD23	2.00	0.43
1:C:364:THR:OG1	1:C:385:THR:HG22	2.19	0.43
1:D:388:THR:CB	4:D:602:HOH:O	2.66	0.43
1:B:75:TRP:CZ2	1:B:83:ARG:HD2	2.54	0.43
1:D:9:LYS:N	1:D:103:GLN:HE22	2.09	0.43
1:D:391:MET:O	1:D:395:LYS:HG3	2.19	0.43
1:A:342:LEU:HD12	1:A:348:GLN:HA	2.01	0.42
1:A:425:LEU:HA	1:A:425:LEU:HD12	1.78	0.42
1:B:277:GLU:O	1:B:312:HIS:HE1	2.01	0.42
1:A:9:LYS:N	1:A:103:GLN:HE22	2.15	0.42
1:B:176:TRP:CZ3	1:B:463:PHE:CD2	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:191:LYS:HD2	1:D:191:LYS:C	2.39	0.42
1:D:387:VAL:HG22	1:D:391:MET:SD	2.60	0.42
1:A:147:LYS:HE3	1:D:77:GLU:O	2.19	0.42
1:B:169:PHE:HB3	1:B:172:VAL:CG1	2.49	0.42
1:C:356:GLU:C	1:C:358:GLY:N	2.72	0.42
1:B:438:HIS:CE1	1:C:438:HIS:CE1	3.04	0.42
1:A:78:MET:SD	1:A:83:ARG:HG2	2.58	0.42
4:A:815:HOH:O	1:B:445:LYS:CE	2.67	0.42
1:D:229:ALA:CA	1:D:232:VAL:HG12	2.50	0.42
1:D:191:LYS:HB2	1:D:231:ILE:CD1	2.50	0.42
1:D:155:HIS:HB3	1:D:484:THR:HG21	2.01	0.42
1:B:9:LYS:N	1:B:103:GLN:HE22	2.15	0.41
1:D:172:VAL:HG13	4:D:607:HOH:O	2.20	0.41
1:D:22:MET:HG3	1:D:221:PRO:HD2	2.02	0.41
1:D:462:PRO:HG3	1:D:478:TYR:CD2	2.55	0.41
1:A:157:PRO:HB3	1:A:184:THR:O	2.19	0.41
1:C:239:LYS:HZ3	1:C:262:HIS:HD2	1.68	0.41
1:A:177:LYS:HZ1	1:A:243:THR:HG22	1.85	0.41
1:A:243:THR:HB	1:A:266:GLU:HB3	2.03	0.41
1:A:137:LYS:HE3	1:C:134:TRP:NE1	2.35	0.41
1:A:260:ILE:HG22	1:A:260:ILE:O	2.21	0.41
1:C:357:GLN:NE2	1:C:361:GLU:OE2	2.54	0.41
1:C:292:ILE:HG21	1:C:403:VAL:HB	2.02	0.41
1:A:165:ILE:CD1	1:A:177:LYS:HG3	2.49	0.41
1:B:263:VAL:CG1	1:B:265:LEU:HG	2.50	0.41
1:B:271:SER:HB3	1:B:426:ALA:O	2.20	0.41
1:B:433:ASN:HD22	1:B:436:THR:H	1.68	0.41
1:B:60:ASP:OD2	1:B:64:LYS:NZ	2.53	0.41
1:B:87:ILE:HG22	1:B:132:ALA:HB2	2.03	0.41
1:A:250:LYS:HE2	1:B:258:GLU:O	2.20	0.41
1:C:359:LYS:HE2	1:C:365:VAL:CG1	2.50	0.41
1:D:153:THR:HA	1:D:487:LYS:O	2.21	0.41
1:D:403:VAL:HG22	1:D:404:VAL:N	2.37	0.40
1:A:127:ASN:OD1	1:A:459:ALA:HB2	2.21	0.40
1:C:395:LYS:HE2	1:C:395:LYS:HB2	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	489/494 (99%)	474 (97%)	15 (3%)	0	100	100
1	B	489/494 (99%)	470 (96%)	19 (4%)	0	100	100
1	C	486/494 (98%)	463 (95%)	21 (4%)	2 (0%)	34	30
1	D	487/494 (99%)	466 (96%)	20 (4%)	1 (0%)	47	44
All	All	1951/1976 (99%)	1873 (96%)	75 (4%)	3 (0%)	47	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	373	LEU
1	C	424	GLY
1	D	166	PRO

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	398/401 (99%)	382 (96%)	16 (4%)	31	29
1	B	398/401 (99%)	380 (96%)	18 (4%)	27	24
1	C	395/401 (98%)	367 (93%)	28 (7%)	14	10
1	D	396/401 (99%)	372 (94%)	24 (6%)	18	14
All	All	1587/1604 (99%)	1501 (95%)	86 (5%)	22	18

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	VAL
1	A	109	ASN
1	A	120	ASP
1	A	121	ILE
1	A	122	SER
1	A	146	SER
1	A	195	GLN
1	A	243	THR
1	A	266	GLU
1	A	296	HIS
1	A	329	LEU
1	A	371	ARG
1	A	373	LEU
1	A	375	LYS
1	A	399	PHE
1	A	453	ASP
1	B	50	VAL
1	B	105	GLU
1	B	109	ASN
1	B	121	ILE
1	B	147	LYS
1	B	195	GLN
1	B	246	THR
1	B	266	GLU
1	B	272	PRO
1	B	296	HIS
1	B	310	ARG
1	B	335	LYS
1	B	351	VAL
1	B	353	ASN
1	B	375	LYS
1	B	387	VAL
1	B	399	PHE
1	B	453	ASP
1	C	27	GLU
1	C	30	SER
1	C	77	GLU
1	C	83	ARG
1	C	98	ARG
1	C	105	GLU
1	C	109	ASN
1	C	115	VAL
1	C	121	ILE

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Mol	Chain	Res	Type
1	C	161	VAL
1	C	166	PRO
1	C	172	VAL
1	C	195	GLN
1	C	283	GLU
1	C	296	HIS
1	C	311	LYS
1	C	329	LEU
1	C	336	GLU
1	C	351	VAL
1	C	360	LYS
1	C	375	LYS
1	C	379	VAL
1	C	385	THR
1	C	387	VAL
1	C	399	PHE
1	C	406	LEU
1	C	412	GLU
1	C	453	ASP
1	D	18	GLU
1	D	77	GLU
1	D	105	GLU
1	D	109	ASN
1	D	121	ILE
1	D	166	PRO
1	D	171	LEU
1	D	188	ILE
1	D	191	LYS
1	D	195	GLN
1	D	266	GLU
1	D	282	GLU
1	D	296	HIS
1	D	311	LYS
1	D	351	VAL
1	D	360	LYS
1	D	373	LEU
1	D	385	THR
1	D	390	ASP
1	D	399	PHE
1	D	404	VAL
1	D	422	SER
1	D	429	VAL

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Mol	Chain	Res	Type
1	D	453	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	A	195	GLN
1	A	214	ASN
1	A	262	HIS
1	A	312	HIS
1	A	325	ASN
1	A	326	ASN
1	A	432	GLN
1	A	433	ASN
1	A	438	HIS
1	A	442	ASN
1	B	55	GLN
1	B	103	GLN
1	B	195	GLN
1	B	214	ASN
1	B	262	HIS
1	B	312	HIS
1	B	325	ASN
1	B	348	GLN
1	B	432	GLN
1	B	433	ASN
1	B	438	HIS
1	B	482	ASN
1	C	103	GLN
1	C	114	GLN
1	C	195	GLN
1	C	214	ASN
1	C	262	HIS
1	C	325	ASN
1	C	326	ASN
1	C	357	GLN
1	C	432	GLN
1	C	433	ASN
1	C	438	HIS
1	C	442	ASN
1	C	482	ASN
1	D	103	GLN

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Mol	Chain	Res	Type
1	D	114	GLN
1	D	195	GLN
1	D	214	ASN
1	D	262	HIS
1	D	312	HIS
1	D	326	ASN
1	D	432	GLN
1	D	433	ASN
1	D	438	HIS
1	D	442	ASN
1	D	482	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 7 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NDP	C	503	-	45,52,52	1.23	5 (11%)	53,80,80	1.40	8 (15%)
3	NDP	D	502	-	45,52,52	1.24	7 (15%)	53,80,80	1.33	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NDP	B	503	-	45,52,52	1.10	5 (11%)	53,80,80	1.34	8 (15%)
3	NDP	A	503	-	45,52,52	1.13	5 (11%)	53,80,80	1.35	8 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NDP	C	503	-	-	3/30/77/77	0/5/5/5
3	NDP	D	502	-	-	3/30/77/77	0/5/5/5
3	NDP	B	503	-	-	4/30/77/77	0/5/5/5
3	NDP	A	503	-	-	4/30/77/77	0/5/5/5

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	503	NDP	C6N-C5N	3.97	1.40	1.33
3	D	502	NDP	C6N-C5N	3.32	1.39	1.33
3	D	502	NDP	C2A-N3A	3.22	1.37	1.32
3	B	503	NDP	C5A-C4A	3.10	1.49	1.40
3	A	503	NDP	C6N-C5N	3.03	1.38	1.33
3	C	503	NDP	C5A-C4A	2.97	1.48	1.40
3	D	502	NDP	C5A-C4A	2.90	1.48	1.40
3	D	502	NDP	C2N-C3N	2.77	1.42	1.34
3	B	503	NDP	C6N-C5N	2.74	1.38	1.33
3	A	503	NDP	P2B-O2B	2.57	1.64	1.59
3	C	503	NDP	C2N-C3N	2.52	1.42	1.34
3	C	503	NDP	O4B-C1B	2.51	1.44	1.41
3	B	503	NDP	C7N-C3N	2.46	1.54	1.48
3	D	502	NDP	C7N-C3N	2.46	1.54	1.48
3	A	503	NDP	C2A-N3A	2.44	1.36	1.32
3	C	503	NDP	C2A-N3A	2.36	1.35	1.32
3	A	503	NDP	C5A-C4A	2.33	1.47	1.40
3	B	503	NDP	P2B-O2B	2.30	1.63	1.59
3	D	502	NDP	P2B-O2B	2.29	1.63	1.59
3	A	503	NDP	C2N-C3N	2.25	1.41	1.34
3	B	503	NDP	C2A-N3A	2.17	1.35	1.32
3	D	502	NDP	O4B-C1B	2.14	1.44	1.41

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	503	NDP	O4D-C1D-N1N	4.42	116.70	108.06
3	A	503	NDP	O4D-C1D-N1N	4.06	116.00	108.06
3	D	502	NDP	O4D-C1D-N1N	4.01	115.90	108.06
3	C	503	NDP	N3A-C2A-N1A	-3.63	123.01	128.68
3	C	503	NDP	C2D-C1D-N1N	-3.49	104.56	113.30
3	A	503	NDP	C4A-C5A-N7A	-3.32	105.94	109.40
3	A	503	NDP	O3X-P2B-O2X	3.29	120.22	107.64
3	B	503	NDP	N3A-C2A-N1A	-3.27	123.56	128.68
3	D	502	NDP	N3A-C2A-N1A	-3.20	123.67	128.68
3	D	502	NDP	C2D-C1D-N1N	-3.14	105.42	113.30
3	A	503	NDP	C2D-C1D-N1N	-2.85	106.17	113.30
3	B	503	NDP	O4D-C1D-N1N	2.70	113.33	108.06
3	B	503	NDP	C2A-N1A-C6A	2.70	123.37	118.75
3	A	503	NDP	N3A-C2A-N1A	-2.67	124.50	128.68
3	B	503	NDP	C1D-N1N-C2N	-2.64	116.72	121.11
3	B	503	NDP	C2D-C1D-N1N	-2.63	106.70	113.30
3	B	503	NDP	O3D-C3D-C2D	2.62	120.29	111.82
3	C	503	NDP	C1B-N9A-C4A	-2.50	122.25	126.64
3	A	503	NDP	C1B-N9A-C4A	-2.39	122.45	126.64
3	D	502	NDP	C4A-C5A-N7A	-2.32	106.98	109.40
3	A	503	NDP	O2N-PN-O1N	2.29	123.56	112.24
3	D	502	NDP	O4D-C4D-C5D	2.23	116.72	109.37
3	C	503	NDP	C3D-C2D-C1D	2.21	105.62	101.43
3	C	503	NDP	C2A-N1A-C6A	2.18	122.48	118.75
3	B	503	NDP	C4A-C5A-N7A	-2.16	107.15	109.40
3	B	503	NDP	C1B-N9A-C4A	-2.13	122.89	126.64
3	C	503	NDP	PN-O3-PA	-2.07	125.72	132.83
3	C	503	NDP	O2X-P2B-O1X	2.06	118.76	110.68
3	A	503	NDP	C1D-N1N-C2N	-2.06	117.68	121.11

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	503	NDP	O4D-C1D-N1N-C2N
3	C	503	NDP	C2N-C3N-C7N-N7N
3	B	503	NDP	O4D-C1D-N1N-C2N
3	B	503	NDP	C2N-C3N-C7N-N7N
3	A	503	NDP	O4D-C1D-N1N-C2N
3	A	503	NDP	C2N-C3N-C7N-N7N
3	D	502	NDP	O4D-C1D-N1N-C2N
3	A	503	NDP	C1B-C2B-O2B-P2B
3	B	503	NDP	C3B-C2B-O2B-P2B

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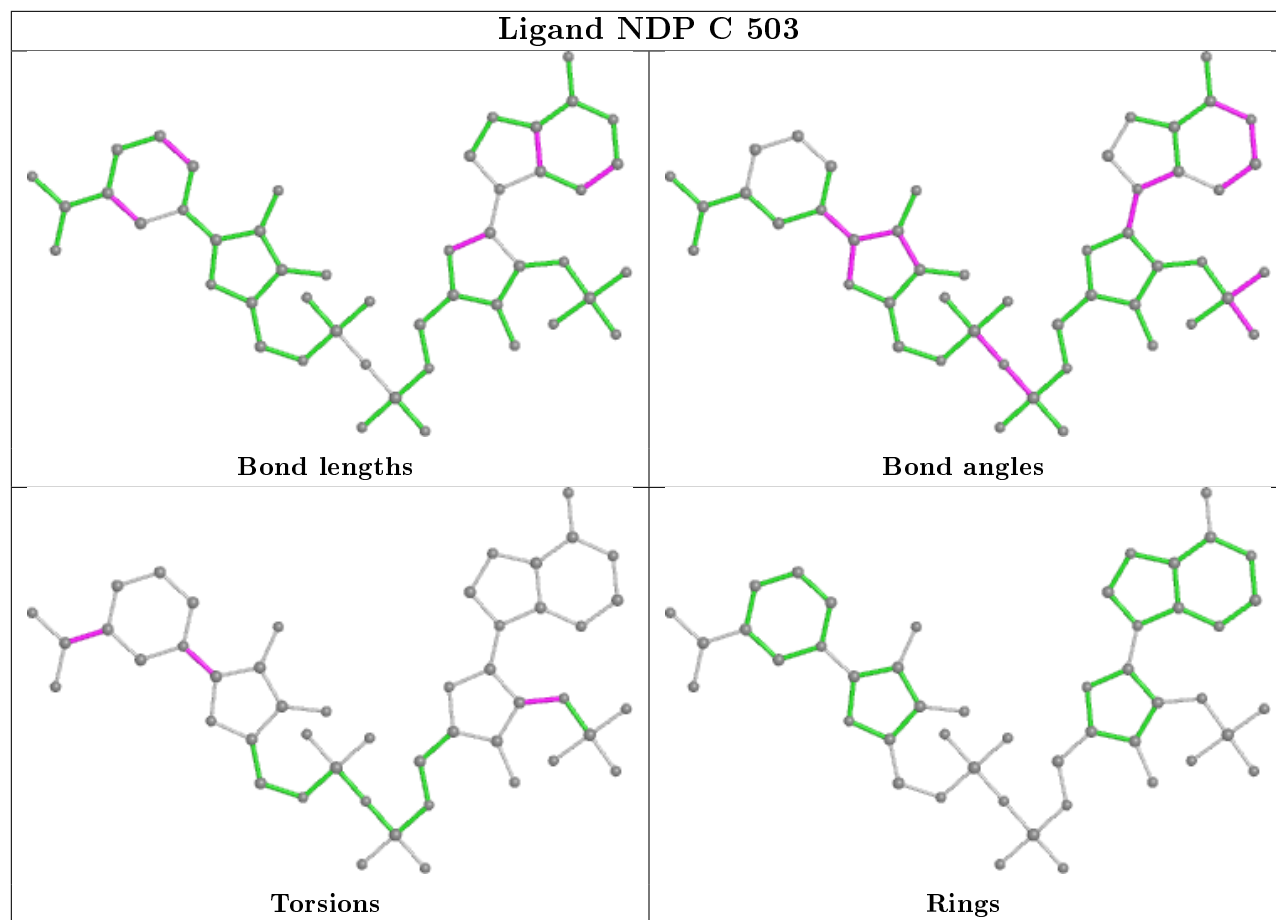
Mol	Chain	Res	Type	Atoms
3	A	503	NDP	C3B-C2B-O2B-P2B
3	B	503	NDP	C1B-C2B-O2B-P2B
3	D	502	NDP	PN-O3-PA-O5B
3	C	503	NDP	C3B-C2B-O2B-P2B
3	D	502	NDP	C4D-C5D-O5D-PN

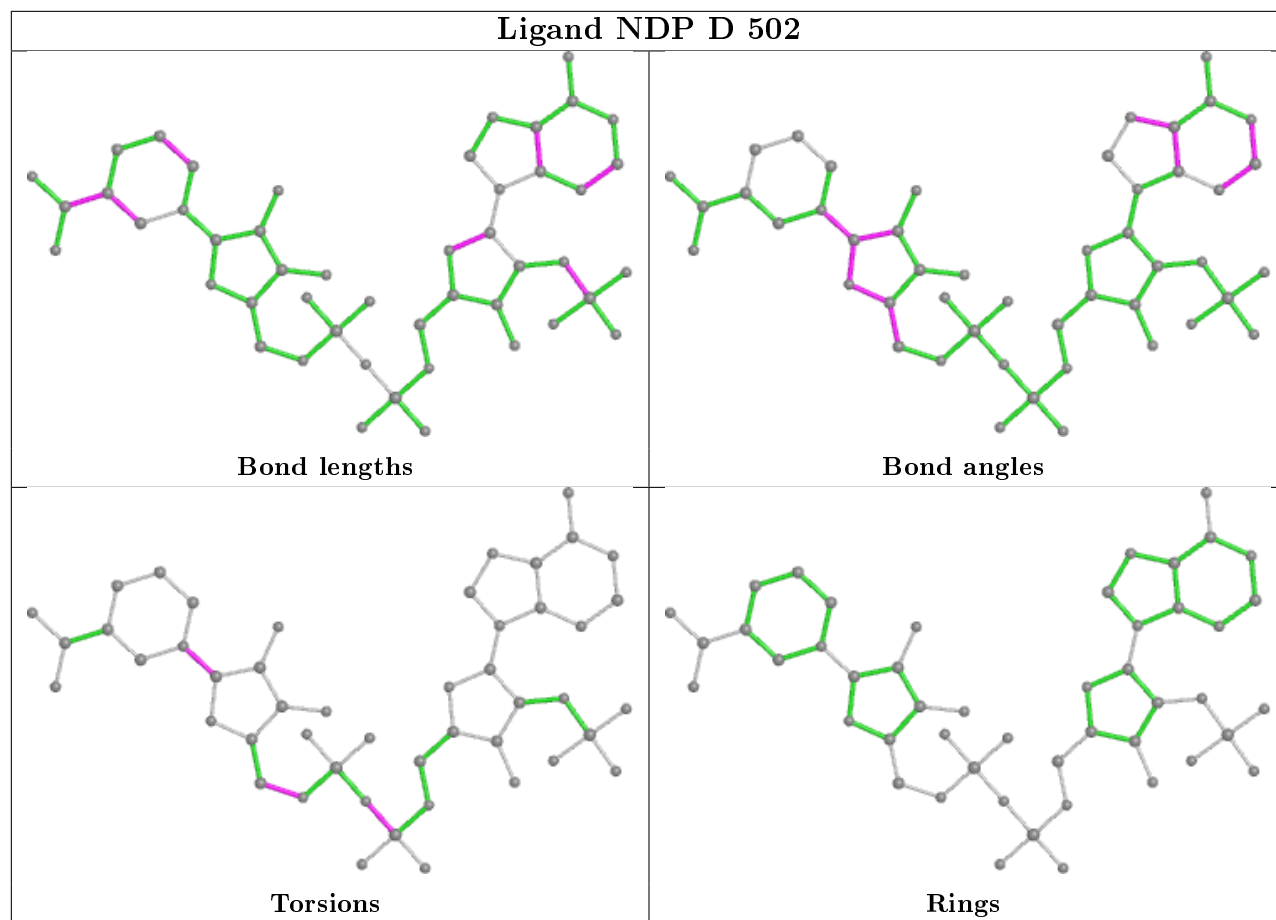
There are no ring outliers.

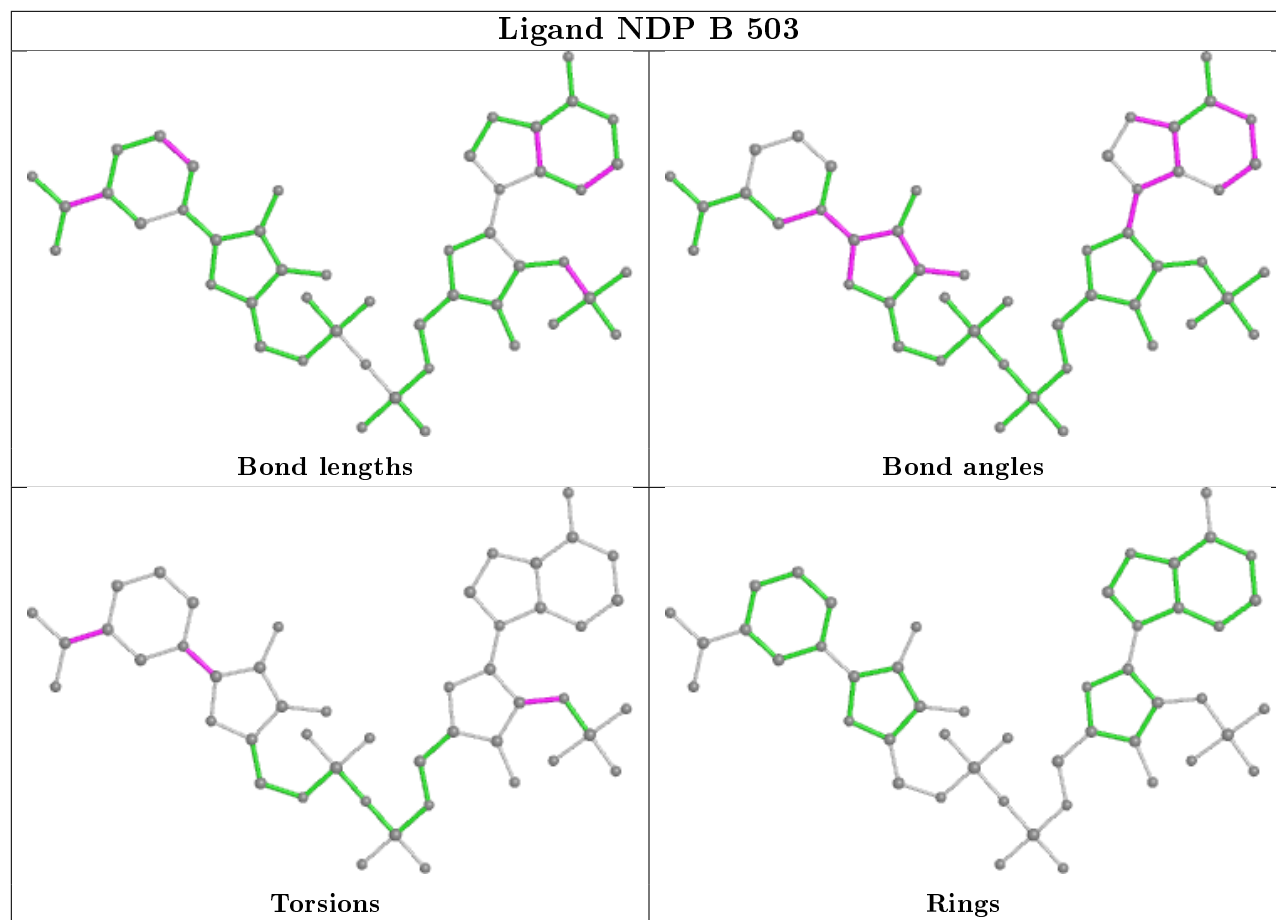
2 monomers are involved in 5 short contacts:

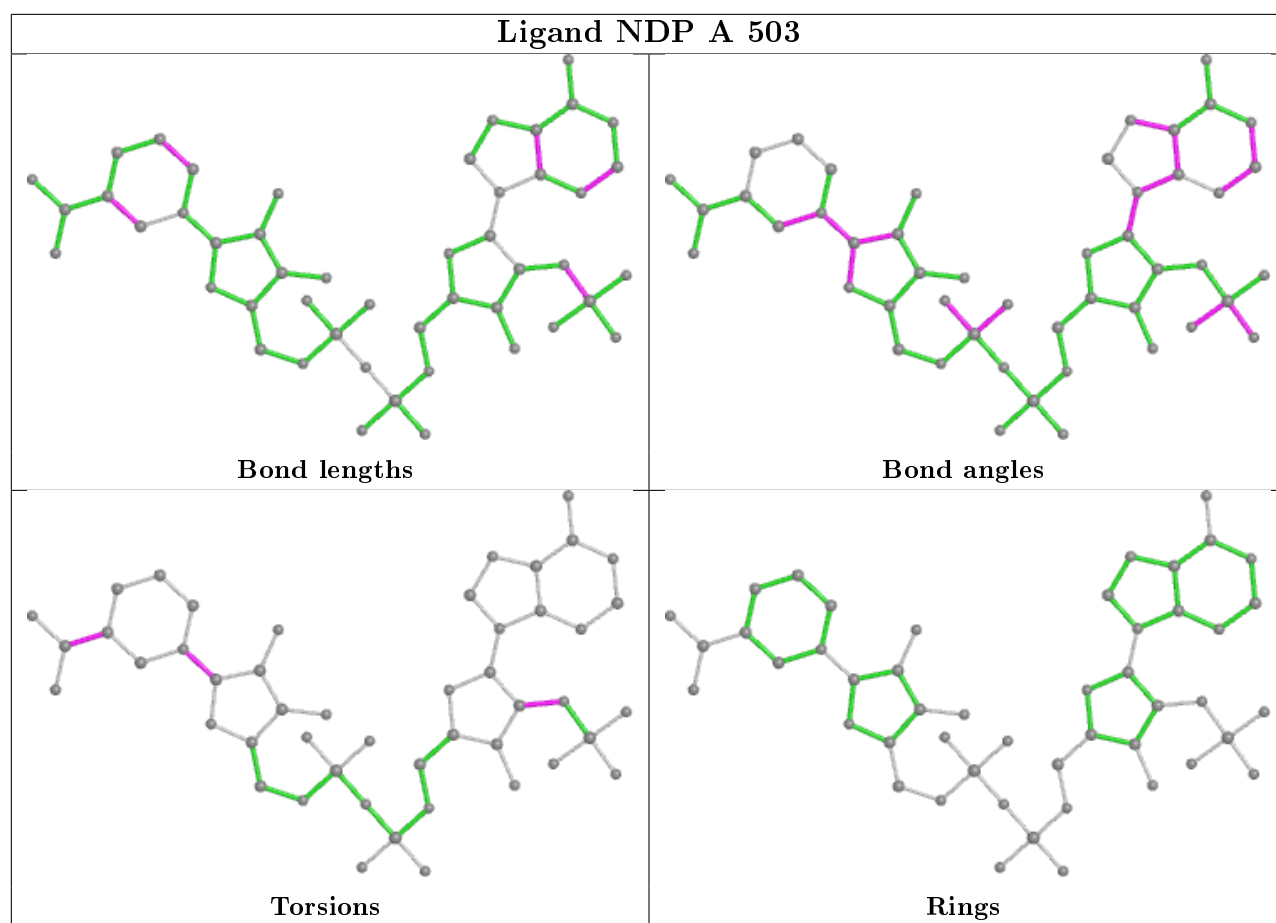
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	502	NDP	4	0
3	A	503	NDP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	491/494 (99%)	-0.37	2 (0%) 92 92	13, 27, 42, 60	0
1	B	491/494 (99%)	-0.25	2 (0%) 92 92	15, 28, 43, 60	0
1	C	488/494 (98%)	-0.06	2 (0%) 92 92	19, 35, 58, 76	0
1	D	489/494 (98%)	-0.17	1 (0%) 95 94	18, 33, 50, 72	0
All	All	1959/1976 (99%)	-0.22	7 (0%) 92 92	13, 30, 50, 76	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	360	LYS	3.0
1	B	176	TRP	2.7
1	C	353	ASN	2.4
1	A	176	TRP	2.4
1	B	463	PHE	2.2
1	D	176	TRP	2.1
1	A	139	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands

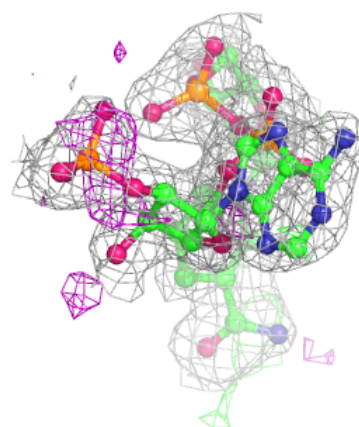
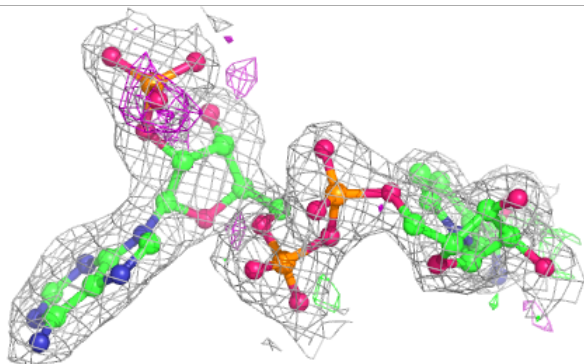
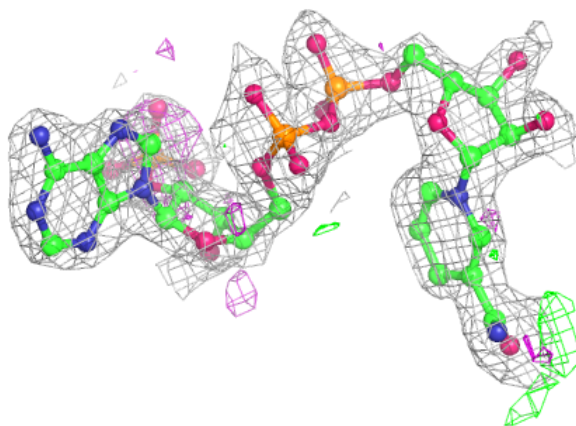
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NA	C	502	1/1	0.85	0.09	40,40,40,40	0
3	NDP	A	503	48/48	0.91	0.12	36,45,51,52	0
3	NDP	D	502	48/48	0.92	0.12	43,54,69,73	0
3	NDP	B	503	48/48	0.94	0.11	32,39,44,46	0
2	NA	D	501	1/1	0.94	0.12	35,35,35,35	0
3	NDP	C	503	48/48	0.94	0.12	41,49,56,60	0
2	NA	B	502	1/1	0.95	0.07	32,32,32,32	0
2	NA	A	502	1/1	0.96	0.05	28,28,28,28	0
2	NA	B	501	1/1	0.96	0.10	27,27,27,27	0
2	NA	C	501	1/1	0.96	0.08	42,42,42,42	0
2	NA	A	501	1/1	0.98	0.07	23,23,23,23	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

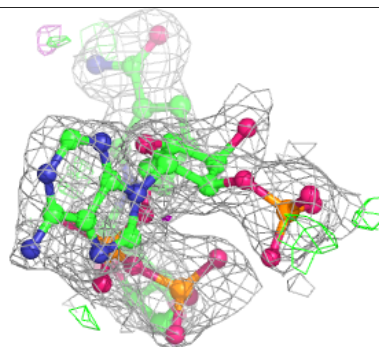
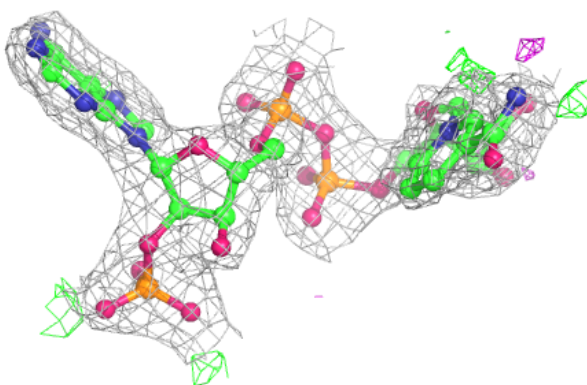
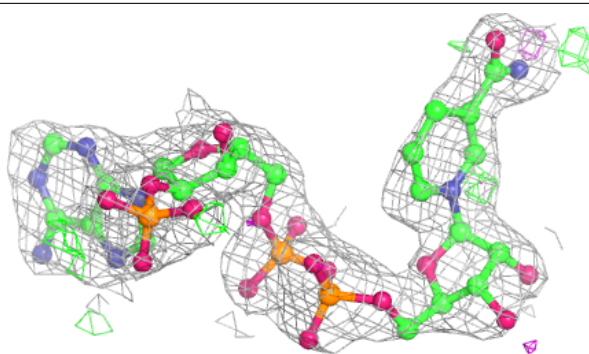
Electron density around NDP A 503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



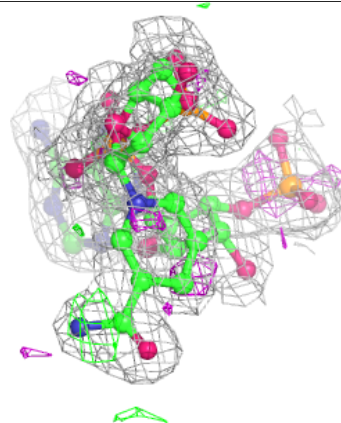
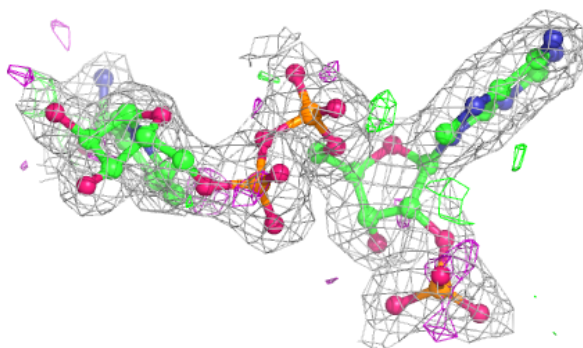
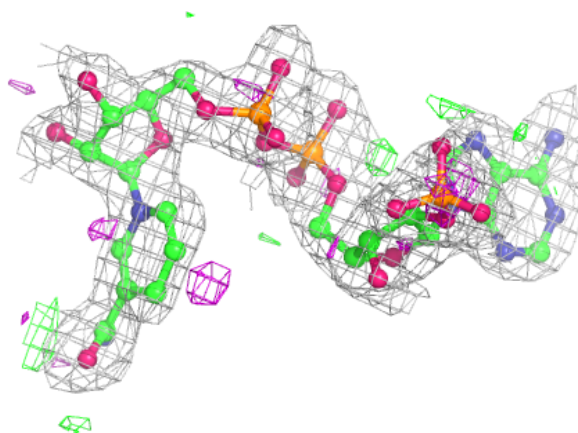
Electron density around NDP D 502:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

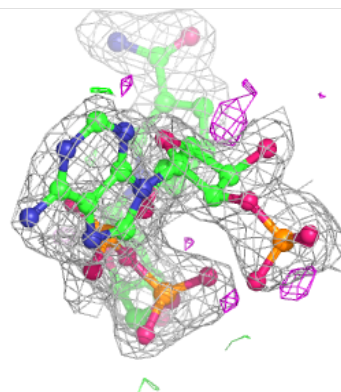
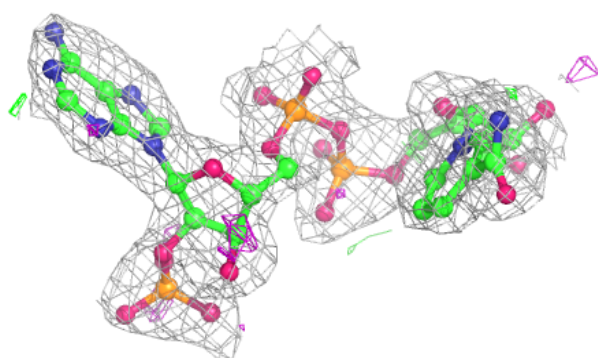
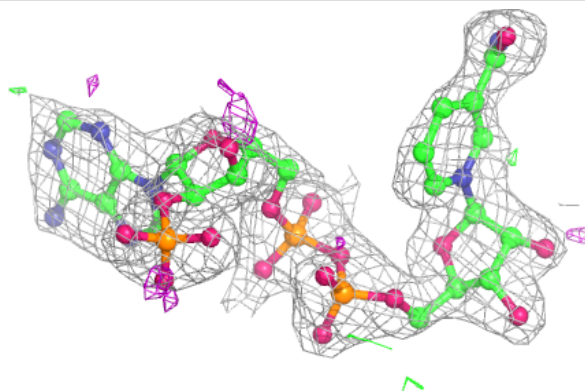


Electron density around NDP B 503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around NDP C 503:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers

There are no such residues in this entry.